

Reducing multi-qubit interactions in adiabatic quantum computation. Part 1: The “deduc-reduc” method and its application to quantum factorization of numbers

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Adiabatic quantum computing has recently been used to factor 56153 [Dattani & Bryans, arXiv:1411.6758] at room temperature, which is orders of magnitude larger than any number attempted yet using Shor’s algorithm (circuit-based quantum computation). However, this number is still vastly smaller than RSA-768 which is the largest number factored thus far on a classical computer. We address a major issue arising in the scaling of adiabatic quantum factorization to much larger numbers. Namely, the existence of many 4-qubit, 3-qubit and 2-qubit interactions in the Hamiltonians. We showcase our method on various examples, one of which shows that we can remove 94% of the 4-qubit interactions and 83% of the 3-qubit interactions in the factorization of a 25-digit number with almost no effort, *without* adding any auxiliary qubits. Our method is not limited to quantum factoring. Its importance extends to the wider field of discrete optimization. Any CSP (constraint-satisfiability problem), psuedo-boolean optimization problem, or QUBO (quadratic unconstrained Boolean optimization) problem can in principle benefit from the “deduction-reduction” method which we introduce in this paper. We provide an open source code which takes in a Hamiltonian (or a discrete discrete function which needs to be optimized), and returns a Hamiltonian that has the same unique ground state(s), no new auxiliary variables, and as few multi-qubit (multi-variable) terms as possible with deduc-reduc.

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I. INTRODUCTION

The quantum algorithm which has perhaps generated the most enthusiasm about quantum computing, is Shor’s algorithm for factoring integers [1, 2]. However, despite being celebrated for more than 20 years, this algorithm has still never been successfully implemented for determining the factors of any integers without using knowledge of the answer to the problem [3, 4]. By using knowledge of the answer to the factorization problem, one can choose a base such that Shor’s algorithm can be implemented with fewer qubits, and by doing this, the algorithm has successfully been implemented for factoring 15 [5–9] and 21 [10]. However, at least 8 qubits are needed for genuinely factoring 15 with Shor’s algorithm [3], and the largest number of qubits ever successfully used in the algorithm was 7 [5].

Adiabatic quantum computing (AQC) has succeeded in factoring much larger numbers with far fewer qubits, without any assumptions about the answer to the factorization problem [4]. The largest number found so far that has been factored by the room-temperature AQC

discrete minimization experiment of [11] is 56153 and it only needed 4 qubits [4]. Furthermore, quantum annealing can be used on AQC algorithms with up to 2048 qubits, which is enough to factor the 100-digit number RSA-100.

Furthermore, quantum annealers have doubled in number of qubits every year between the 4-qubit Calypso machine in 2005 and the 2048-qubit Washington machine in 2015 (a phenomenon analogous to Moore’s law and known as “Rose’s Law”). RSA-220, which is the smallest RSA number that has not yet been factored by any computer (whether quantum or classical), would need only ~ 5000 qubits to factor successfully with the AQC algorithm of [4], which would be well within the 8192-qubit capacity of a 2017 quantum annealer if Rose’s law continues to hold as it has done for the last 10 years.

However, there is a major obstacle holding back such quantum annealers with colossal numbers of qubits, from implementing the AQC factoring algorithm. All such quantum annealing devices reported to date can only implement AQC algorithms which have at most 2-qubit interactions in their Hamiltonian. The algorithm which can factor RSA-220 with ~ 5000 qubits has a Hamiltonian with many 4-qubit and 3-qubit interactions. In 2007 Schaller and Schutzholt devised an alternate AQC algorithm for factoring integers, which only has up to 2-qubit interactions in the Hamiltonian,

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and whose Hamiltonian's spectral width (which is used for determining the runtime of the annealing) increases only polynomially in the number being factored [12].

The problem with this AQC algorithm that uses at most 2-qubit interactions and whose spectral width only increases polynomially, is that it requires adding a large number of auxiliary qubits (27 225 for RSA-100, and 133 225 for RSA-220). In this paper we present a method, called "deduc-reduc" for reducing the number of 4-qubit and 3-qubit terms in the AQC Hamiltonian *without* adding auxiliary qubits.

While the motivation for this work was the problem of factoring numbers using AQC, deduc-reduc can be used for a wider range of discrete optimization problems such as constraint satisfaction problems (CSPs) and pseudo-Boolean optimization problems, and problems arising in the field of artificial intelligence/neural networks [13]. All of these problems can benefit from quantum annealing because of the capability for quadratic speed-up over simulated annealing [14]. Quantum annealing has also recently been shown to be able to provide exponential speed-up for some specific discrete optimization problems [15], and the potential for speeding up more general discrete optimization problems is an active area of research.

It has also been shown that AQC can simulate any circuit-based quantum algorithm with only polynomial overhead [16, 17]. Therefore, apart from the exponential speed-up offered for many classes of problems, AQC can provide polynomial speed-up over the best classical 3-SAT algorithms [?] and other CSPs [18], and can provide exponential speed-up for combinatorial optimiza-

tion problems for which an approximate solution is sufficient [19].

II. A QUICK EXAMPLE

It has been shown with concrete examples in many papers [4, 11, 12, 20] that integer factorization is equivalent to solving a system of binary equations such as:

$$x_1 + x_2 + x_3 = 1 \quad (1)$$

$$x_1 x_4 + x_2 x_5 = x_3 \quad (2)$$

$$x_1 + 2x_2 = x_3 + 2x_4 \quad (3)$$

which is equivalent to finding the minimum of an objective function formed by subtracting the right hand side of each equation from its left, squaring, and summing (and remembering that the square of a binary variable is itself):

$$H = (x_1 + x_2 + x_3 - 1)^2 + (x_1 x_4 + x_2 x_5 - x_3)^2 + \quad (4)$$

$$(x_1 + 2x_2 - x_3 - 2x_4)^2 \quad (5)$$

$$= 2x_1 x_2 x_4 x_5 - 2x_1 x_3 x_4 - 2x_2 x_3 x_5 - 2x_2 x_3 + 6x_1 x_2 \quad (6)$$

$$- 3x_1 x_4 - 8x_2 x_4 + x_2 x_5 + 3x_2 + 4x_3 x_4 + x_3 + 4x_4 + 1 \quad (7)$$

If we represent each variable x_i as a qubit based on a Pauli spin matrix in its own Hilbert space:

$$x_i = \frac{1}{2} (1 - \sigma_z^{(i)})^2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (8)$$

and each term of Eq. 6 using left Kronecker products (or "tensor products") in the Hilbert space of all qubits, for example:

$$2x_1 x_2 x_4 x_5 = 2x_1 x_2 \mathbf{1}_3 x_4 x_5 = 2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (9)$$

$$= \text{diag}(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 2), \quad (10)$$

we see quickly that the objective function of Eq. 6 can be represented as a diagonal 32×32 Hamiltonian matrix:

$$H = \text{diag}(1, 1, 5, 5, 2, 2, 10, 10, 4, 5, 0, 1, 3, 2, 3, 2, 1, 1, 2, 2, 2, 2, 5, 5, 10, 11, 3, 6, 9, 8, 4, 5).$$

The lowest eigenvalue is clearly 0, and it is at position:

$$\text{diag}(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) = |x_1 = 0, x_2 = 1, x_3 = 0, x_4 = 1, x_5 = 0\rangle. \quad (11)$$

This may seem like an unnecessary extra complication to find the minimum, especially since if we have N variables, it involves representing all 2^N values of H and then searching for the lowest one. However, since the lowest eigenvalue of a Hamiltonian corresponds to its ground state, the minimum of a 2^N variable system can be found simply by connecting N qubits together

with appropriate energies and coupling strengths, then finding the ground state of this system. This avoids having to evaluate the function 2^N times. But it is *much* harder to couple three qubits together as in the cubic term $2x_1 x_2 x_3$, than it is to couple two qubits together as in the quadratic terms, which is of course still harder than not having to enforce any couplings (but if only

linear terms exist, the problem can be solved trivially by setting all negative terms to 1 and positive terms to 0). Likewise, even if solving this problem on a classical computer, multi-variable (or multi-qubit) terms make the problem *much* more difficult, and it is desirable to eliminate any terms containing more than 2 variables, since this would transform the problem into a quadratic unconstrained Boolean optimization (QUBO) problem, whereby we can use many beautiful algorithms and results such as the fact that the solution can be found in polynomial time if all quadratic terms are negative [21–24]. Furthermore, it is also desirable to eliminate as many quadratic terms as possible.

A. The method

We now demonstrate how deduc-reduc can be used to eliminate multi-qubit interactions (or high-order terms).

From Eq. 1 alone we can make the *deductions*:

$$x_1x_2 = x_2x_3 = x_3x_1 = 0 \quad (12)$$

since the LHS of Eq. 1 cannot be greater than 1, and this would not be true if any of the products in Eq. 12 were 1.

Naive substitution

Suppose that we substituted Eq. 12 back into H :

$$H = -3x_1x_4 - 8x_2x_4 + x_2x_5 + 3x_2 + 4x_3x_4 + x_3 + 4x_4 + 1. \quad (13)$$

Then we find that while $H(0, 1, 0, 1, 0) = 0$ matches the original Hamiltonian as required, we have also introduced a new state with $H = -3$ and another for which $H = -2$. This is a problem, because if the minimum is not 0, then the ground state does *not* encode the solution to Eqs 1-3, which is the integer factorization problem we want to solve.

Deduc-reduc

Instead, we can look at each term we would like to substitute Eq. 12 into, and calculate an associated error term.

We want an error term such that it is equal to 0 if $x_1x_2 = 0$ and strictly greater than 0 if $x_1x_2 \neq 0$. In this particular example, we can take x_1x_2 to be our error term and similarly for x_2x_3 and x_3x_1 . We will now work through the rest of this example in order to illustrate the method, but a general formulation can be found in Section III.

We have three cubic/quartic terms to consider:

1. $2x_1x_2x_4x_5$. Here we make use of the judgment $x_1x_2 = 0$. For any state, $2x_1x_2x_4x_5$ can only evaluate to 0 or 2. In the former case, a straight substitution does not make any difference to the value of

H and setting the term to 0 is permissible. If the term evaluates to 2 (i.e. all variables are equal to 1) and we perform a straight substitution, we are taking 2 away from the energy of the state. This may introduce new states with $H = 0$ or even negative valued states. To compensate for this, we add $2x_1x_2$ back on to the original Hamiltonian to preserve the original value of H . We have then made the transformation $2x_1x_2x_4x_5 \rightarrow 2x_1x_2$. While this step may add 2 to the original energy of a state, the important detail is that we know this will not happen for any ground states.

2. $-2x_1x_3x_4$. This can only take the values 0 or -2 . In the first case, a straight substitution makes no difference. In the second, a straight substitution for 0 would add 2 to the value of the incorrect state, which is safe to do, (it is even desirable, since increasing the energy gap between the ground and excited states can allow the ground state to be found quicker by annealing or adiabatic evolution methods, and the power to manipulate the energy landscape like this is the subject of our forthcoming paper [25]). Hence we can make the transformation $-2x_1x_3x_4 \rightarrow 0$.
3. $-2x_2x_3x_5$. As with case 2, we make the transformation $-2x_2x_3x_5 \rightarrow 0$.

Bringing the above substitutions together we get a Hamiltonian with the *same* number of qubits as before, but has *no* 4-qubit (quartic) nor 3-qubit (cubic) terms, and whose only ground state is precisely the ground state of the original Hamiltonian:

$$H = 8x_1x_2 - 2x_2x_3 - 3x_1x_4 - 8x_2x_4 + x_2x_5 + \quad (14)$$

$$3x_2 + 4x_3x_4 + x_3 + 4x_4 + 1. \quad (15)$$

A quick numerical check shows that our new Hamiltonian has a single zero at exactly the original solution as required. We have therefore used our *deductions* in Eq. 12 to do a *reduction* of the 4-qubit and 3-qubit terms.

Removing quadratic terms

Notice that when the coefficient of a term was negative, we were able to perform a straight substitution, as doing so only added to the energy of a state and no error term was needed. This can also be used to eliminate quadratic terms like $-2x_2x_3$, to provide extra simplification. Our final Hamiltonian is then:

$$H = 8x_1x_2 - 3x_1x_4 - 8x_2x_4 + x_2x_5 + 3x_2 + 4x_3x_4 + x_3 + 4x_4 + 1. \quad (16)$$

Note that in general we can remove quadratic terms by following the method described in Section III. However, this is

Table I. The three examples used to illustrate the power of deduc-reduc for removing multi-qubit interactions.

Example	Product	Length of product in binary
1	455937533473	40
2	292951160076082381	60
3	1208925727750433490141601	80

difficult in practice because any deduction must be at least quadratic (else we perform a straight substitution) and requires an appropriate error term.

B. Performance of deduc-reduc on large examples

We now consider the performance of deduc-reduc on Hamiltonians whose ground states encode the prime factors to larger numbers, displayed in Table I.

For each example, we generate the carry equations that express the factorization and then form the Hamiltonian as in [4, 20]: this is our starting Hamiltonian H_0 . Next, we perform simple logical deductions to solve for the most obvious variables (as in Eq. 12 and the Supplementary Material of [11]), using no enumeration of solutions or deduc-reduc machinery. We call this reduced Hamiltonian H_1 .

Finally we perform searches through the state space by enumerating plausible solutions and looking for patterns that can be used by deduc-reduc. We perform a breadth-first search that halts when it has found more than n plausible solutions. We call the Hamiltonian formed using deduc-reduc with the deductions from such a search H_n .

Enumerating all possible solutions is akin to doing a brute force search for the minimum, so of course it would make no sense to run this algorithm for n anywhere close to the total size of the search space 2^N where N is the number of qubits in the Hamiltonian. However, in the examples from Table I, we show in Table II that with n vastly smaller than 2^N , we can still eliminate a significant number of multi-qubit interactions¹. No deduc-reduc example we present takes more than a few hours of CPU time on an average laptop, and 1000 states takes just a few seconds. The code is written in Python with scope for optimization and parallelization.

¹ While the factorization problem can be directly solved by brute force using $2^m < 2^N$ trials, where m is the bit-length of the number we wish to factorize, most discrete optimization problems will not have this feature, so the brute force search to solve the problem will generally require 2^N trials where N is the number of variables. Furthermore, the number of states in our search is still vastly fewer than even 2^m .

In Example 1 we are unable to make a big difference in the number of multi-qubit interactions because both the simple judgments and local searches are unable to find many solutions or deductions that are useful for deduc-reduc. In Example 2, the large improvement in the qubit profile comes from the power of simple judgments, which leaves little ‘easy’ work for the search and deduc-reduc to do afterwards. The remarkable success of deduc-reduc in Example 3 stems from the effectiveness of the breadth-first search’s ability to find patterns. The factors that affect the performance of the simple judgments and the breadth-first search are a potential area for future research though we believe it is related to the distribution of 0s and 1s in the binary representations of the factors.

III. GENERAL TREATMENT

A. General formulation

Let \underline{x} be a binary string of length n . Suppose we have a general Hamiltonian $H(\underline{x})$ and a deduction $f(\underline{x}) = g(\underline{x})$ that is true for all ground states, and f, g are polynomials with the degree of g strictly less than the degree of f . Suppose further that we are able to write $H(\underline{x}) = q(\underline{x})f(\underline{x}) + r(\underline{x})$ for some polynomials $q \neq 0$ and r . Then substitution of f for g would give a new polynomial with fewer high order terms.

To allow us to perform this substitution and preserve the global minima, we add an error term $\lambda C(\underline{x})$ of sufficient magnitude to compensate for the substitution. If we start with the deduction “ $f(\underline{x}) = g(\underline{x})$ for all minima \underline{x} ” and form a corresponding error term $C = (f - g)^2$, we define the new polynomial:

$$H'(\underline{x}) = q(\underline{x})g(\underline{x}) + r(\underline{x}) + \lambda C(\underline{x}) \quad (17)$$

$$= q(\underline{x})g(\underline{x}) + r(\underline{x}) + \lambda(f - g)^2 \quad (18)$$

where $|q(\underline{x})| \leq \lambda$ for all states \underline{x} . We claim that H' has exactly the same minima as H , and no new minima, and we prove it in the next sub-section.

B. Proof of formulation

To show that this $H'(x)$ has the required properties, we condition on whether or not a state \underline{x} is a ground state of the original Hamiltonian.

1. If \underline{x} is a ground state then $f(\underline{x}) = g(\underline{x})$ and $C(\underline{x}) = (f - g)^2 = 0$ so we have

$$H'(\underline{x}) = q(\underline{x})g(\underline{x}) + r(\underline{x}) + \lambda C(\underline{x}) \quad (19)$$

$$= q(\underline{x})f(\underline{x}) + r(\underline{x}) \quad (20)$$

$$= H(\underline{x}) \quad (21)$$

as required.

Table II. Performance of deduc-reduc on the three examples from Table I.

455937533473 = 524309 × 869597 = 10000000000000010101 × 11010100010011011101						
Hamiltonian	# of qubits	# of deductions	4-qubit terms	3-qubit terms	2-qubit terms	1-qubit terms
Original, H_0	174	-	1785	3318	1783	150
Simple Judgments, H_1	148	-	1750	2915	1407	128
Reduction with 100 states, H_{100}	146	88	1645	2828	1404	128
Reduction with 1000 states, H_{1000}	144	121	1645	2794	1411	126
Reduction with 10 000 states, $H_{10\,000}$	141	131	1645	2704	1362	123
Reduction with 100 000 states, $H_{100\,000}$	138	242	1645	2591	1370	120
292951160076082381 = 539152967 × 543354443 = 100000001000101101001001000111 × 100000011000101110111001001011						
Hamiltonian	# of qubits	# of deductions	4-qubit terms	3-qubit terms	2-qubit terms	1-qubit terms
Original, H_0	294	-	6930	8816	3541	268
Simple Judgments, H_1	200	-	3686	5061	2222	180
Reduction with 100 states, H_{100}	199	100	3388	4942	2193	180
Reduction with 1000 states, H_{1000}	199	160	3388	4924	2192	180
Reduction with 10 000 states, $H_{10\,000}$	189	111	3388	4860	2074	173
Reduction with 100 000 states, $H_{100\,000}$	185	129	3388	4747	1992	169
1208925727750433490141601 = 1099511555521 × 1099511616481						
11111111111111111111111101110010111000001 × 1111111111111111111111111101001111100001						
Hamiltonian	# of qubits	# of deductions	4-qubit terms	3-qubit terms	2-qubit terms	1-qubit terms
Original, H_0	430	-	17575	17762	5891	382
Simple Judgments, H_1	367	-	16133	16005	5256	367
Reduction with 100 states, H_{100}	333	56	8469	14203	6881	327
Reduction with 1000 states, H_{1000}	257	289	1449	3649	6180	257
Reduction with 10 000 states, $H_{10\,000}$	253	285	1449	3565	6106	253
Reduction with 100 000 states, $H_{100\,000}$	236	236	1142	2961	5732	236

2. If \underline{x} is not a solution, we have that $|q(\underline{x})| \leq \lambda$, by construction, and $|g(\underline{x}) - f(\underline{x})| \leq (g(\underline{x}) - f(\underline{x}))^2$, as we are dealing with polynomials taking integer values. Hence

$$0 \leq q(\underline{x})(g(\underline{x}) - f(\underline{x})) + \lambda(g(\underline{x}) - f(\underline{x}))^2. \quad (22)$$

Then,

$$H'(\underline{x}) = q(\underline{x})g(\underline{x}) + r(\underline{x}) + \lambda C(\underline{x}) \quad (23)$$

$$= (q(x)f(x) + r(x)) + q(x)(g(x) - f(x)) + \quad (24)$$

$$\lambda C(\underline{x}) \quad (25)$$

$$= H(\underline{x}) + q(\underline{x})(g(\underline{x}) - f(\underline{x})) + \lambda(g(\underline{x}) - f(\underline{x}))^2 \quad (26)$$

$$> 0$$

since $H(\underline{x}) > 0$.

Hence $H(\underline{x}) = 0$ if and only if $H'(\underline{x}) = 0$.

C. Calculation of λ

While maximizing an arbitrary integer valued polynomial in n variables might seem suspiciously similar to the original problem, we only need an upper bound. Such a bound can quickly be found by the triangle inequality. However, this might lead to much larger coefficients than are needed. It is perfectly permissible to split up $q(\underline{x})$ and apply repeatedly, as we did in our example to find Hamiltonian 14.

In the most general case, λ can be picked even more precisely depending on the f, g, C and q , as long as the following inequality is satisfied:

$$0 \leq q(\underline{x})(g(\underline{x}) - f(\underline{x})) + \lambda C(\underline{x}) \text{ for all states } \underline{x}. \quad (27)$$

IV. CONCLUSION

For any discrete optimization problem, we have presented a method (called “deduc-reduc”) that can re-formulate the objective function such that without

adding auxiliary variables, the new objective function has fewer high-order terms. Any input that minimizes the original objective function also minimizes the new one, and no new inputs can minimize the objective function. This can be used to reduce a high-order objective function into an easier one, such as a quadratic Boolean optimization problem (QUBO). On our examples for integer factorization, we were able to remove thousands of quartic and cubic terms in a few seconds on a laptop. We provide an open source code with sample input files in [26].

The method we presented can also be used to turn a target Hamiltonian in adiabatic quantum computation (AQC), without adding auxiliary qubits, into one with equivalent unique ground states, but with only 2-qubit terms (for implementations using, for example SQUID-based quantum annealing devices that cannot yet couple more than 2 qubits [27]) or low enough order terms for other AQC-like implementations such as NMR-based devices which can implement 3- and 4-qubit interactions with some more effort [11].

The method we presented here can also be used to manipulate the energy landscape of a Hamiltonian without changing the unique ground states. Particu-

larly, it can be used to move low-lying excited states (local minima of the objective function) away from the ground state (global minimum of the objective function) and to adjust the Hamiltonian's spectral width (range of the objective function) without adding more qubits. This would allow for adjusting the size of the spectral gap between the ground and first excited states of the target Hamiltonian, and therefore it can be used to decrease the runtime of the adiabatic quantum computation, and to also speed-up conventional discrete optimization calculations such as simulated annealing. This is the subject of a forthcoming publication [25].

Finally, this is the first paper of a 2-part series on techniques for reducing multi-variable terms in discrete optimization problems. The second method is called "split-reduc" and is presented in [28] with examples focused on the quadratization of Hamiltonians used for AQC-based determination of Ramsey numbers [29, 30].

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